

### Active-Set Methods for Large-Scale NLP

GIAN Short Course on Optimization: Applications, Algorithms, and Computation

Sven Leyffer

Argonne National Laboratory

September 12-24, 2016



### Outline

- Introduction and Motivation
- 2 Large-Scale Active-Set Methods for QP
  - Augmented Lagrangians for QPs
  - Filter Methods for Augmentd Lagrangian QPs
- 3 Large-Scale Active-Set Methods for NLP
  - Augmented Lagrangian Filter Method
  - Outline of Convergence Proof
  - Outlook and Conclusions

## Active Set Methods for Nonlinear Programming (NLP)

Nonlinear Program (NLP)

minimize 
$$f(x)$$
 subject to  $c(x) = 0$ ,  $x \ge 0$ 

where f, c twice continuously differentiable

### Definition (Active Set)

Active set:  $A(x) = \{i \mid x_i = 0\}$ 

Inactive set:  $\mathcal{I}(x) = \{1, \dots, n\} - \mathcal{A}(x)$ 

For known optimal active set  $A(x^*)$ , just use Newton's method

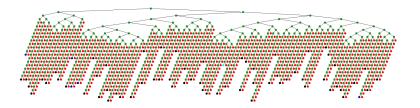
Goal: develop robust, fast, parallelizable active-set methods



# Active Set Methods for Nonlinear Programming (NLP)

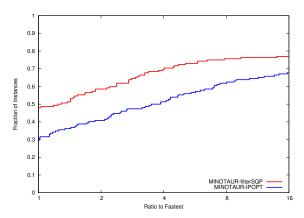
Motivation: mixed-integer nonlinear optimization:  $x_i \in \{0,1\}$ 

- solve NLP relaxation  $x_i \in [0, 1]$
- branch on  $\hat{x}_i \notin \{0,1\}$  ... two new NLPs:  $x_i = 0$  or  $x_i = 1$
- solve sequence of closely related NLPs



Branch-and-bound solves millions of related NLPs ...

### Active-Set vs. Interior-Point Solvers in MINLP



### MINOTAUR with FilterSQP vs IPOPT: CPU time

- FilterSQP warm-starts much faster than IPOPT
- similar results for BONMIN (IBM/CMU) solver



## Large-Scale Active-Set Methods

#### Goal of This Lecture

Towards scalable active-set methods for nonlinear optimization

#### Two Approaches for Large-Scale Active-Set Methods

- Develop methods for large-scale QP
  - ullet Use within SQP framework  $\Rightarrow$  readily understood
  - Should work for indefinite QPs
  - Must allow large changes to active set ... not pivoting
  - Should be scalable ... i.e. matrix-free linear algebra
- ② Develop methods for large-scale NLP
  - Ensure suitable for matrix-free linear algebra
  - Properly combine step-computation and globalization strategy

### Outline

- Introduction and Motivation
- 2 Large-Scale Active-Set Methods for QP
  - Augmented Lagrangians for QPs
  - Filter Methods for Augmentd Lagrangian QPs
- 3 Large-Scale Active-Set Methods for NLP
  - Augmented Lagrangian Filter Method
  - Outline of Convergence Proof
  - Outlook and Conclusions



## Recall: Projected Gradient for Box Constrained QPs

Simpler box constrained QP ...

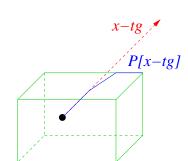
minimize 
$$\frac{1}{2}x^T H x + g^T x =: q(x)$$
  
subject to  $l \le x \le u$ 

Projected steepest descent  $P[x - \alpha \nabla q(x)]$ 

- piecewise linear path
- large changes to A-set
  ... but slow (steepest descent)

$$x^c$$
 Cauchy point  $\equiv$  first minimum of  $q(x(\alpha))$ , for  $\alpha \geq 0$ 

Theorem: Cauchy points converge to stationary point.



# Projected Gradient & CG for Box Constrained QPs

 $x^0$  given such that  $l \le x^0 \le u$ ; set k = 0

#### WHILE (not optimal) BEGIN

- find Cauchy point  $x_k^c$  & active set  $A(x_k^c) := \{i | [x_k^c]_i = I_i \text{ or } u_i\}$
- ② (approx.) solve box QP in subspace  $\mathcal{I} := \{1, \dots, n\} \mathcal{A}(x_k^c)$

minimize 
$$\frac{1}{2}x^T H x + g^T x$$
  
subject to  $1 \le x \le u$   
 $x_i = [x_k^c]_i, \forall i \in \mathcal{A}(x_k^c)$ 

for 
$$x^{k+1}$$
; set  $k = k + 1$ 

#### **END**

Cauchy point ⇒ global convergence ... but faster due to CG



### How to Include $A^Tx = b$ ?

Projection onto box is easy, but tough for general QP

$$P_{QP}[z] = \begin{cases} \underset{x}{\text{minimize}} & (x - z)^T (x - z) \\ \text{subject to } A^T x = b \\ & l \le x \le u \end{cases}$$

... as hard as original QP! ... Idea: project onto box only

 $\Rightarrow$  subspace solve  $H_{\mathcal{I},\mathcal{I}}x_{\mathcal{I}}=...$  becomes solve with KKT system

$$\begin{bmatrix} H_{\mathcal{I},\mathcal{I}} - A_{:,\mathcal{I}} \\ A_{:,\mathcal{I}}^T \end{bmatrix} \begin{pmatrix} x_{\mathcal{I}} \\ y \end{pmatrix} = \dots$$

Which gradient / merit function in Cauchy step?



## The Augmented Lagrangian

[Arrow & Solow:58], [Hestenes:69], [Powell:69]

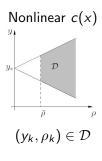
minimize 
$$L(x, y_k, \rho_k) = f(x) - y_k^T c(x) + \frac{1}{2} \rho_k ||c(x)||^2$$

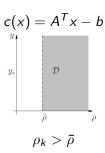
- As  $y_k \to y_*$ :  $\bullet x_k \to x_*$  for  $\rho_k > \bar{\rho}$ 
  - No ill-conditioning, improves convergence rate
- An old idea for nonlinear constraints ... smooth merit function
- Poor experience with LPs (e.g., MINOS vs. LANCELOT)
- But special structure of LPs (and QPs) not fully exploited

$$f(x) = \frac{1}{2}x^{T}Hx + g^{T}x$$
 &  $c(x) = A^{T}x - b$ 



## Augmented Lagrangian for Linear Constraints





 $\forall (\rho, y) \in \mathcal{D}$ , minimize  $L(x, y, \rho)$  has unique solution  $x(y, \rho)$ :

- bound constrained augmented Lagrangian converges
- Hessian  $\nabla^2_{xx} L(x, y, \rho)$  is positive definite on optimal face
- $\bar{\rho} \approx 2\|H_*\| / \|A_*A_*\| \Rightarrow$  convergence

### WHILE (not optimal) BEGIN

• Find  $\omega_k \searrow 0$  optimal solution  $x_k^c$  of

minimize 
$$\frac{1}{2}x^{T}Hx + g^{T}x - y^{T}(A^{T}x - b) + \frac{1}{2}\rho_{k}||A^{T}x - b||^{2}$$

- ② Find  $\mathcal{A}(x_k^c)$  & estimate penalty  $\bar{\rho} = 2 \|H_{\mathcal{I}}\| / \|A_{\mathcal{I}}A_{\mathcal{I}}^T\|$
- **3** IF  $\bar{\rho} > \rho_k$  THEN update  $\rho_{k+1} = \bar{\rho}$  & CYCLE ELSE update multiplier:  $y_k^c = y_k \rho_k (A^T x_k^c b)$

### WHILE (not optimal) BEGIN

• Find  $\omega_k \searrow 0$  optimal solution  $x_k^c$  of

minimize 
$$\frac{1}{2}x^{T}Hx + g^{T}x - y^{T}(A^{T}x - b) + \frac{1}{2}\rho_{k}||A^{T}x - b||^{2}$$

- ② Find  $\mathcal{A}(x_k^c)$  & estimate penalty  $\bar{\rho} = 2 \|H_{\mathcal{I}}\| / \|A_{\mathcal{I}}A_{\mathcal{I}}^T\|$
- **3** IF  $\bar{\rho} > \rho_k$  THEN update  $\rho_{k+1} = \bar{\rho}$  & CYCLE ELSE update multiplier:  $y_k^c = y_k \rho_k (A^T x_k^c b)$
- Solve equality QP in subspace  $\rightarrow (\Delta x_{\mathcal{I}}, \Delta y)$

$$\begin{bmatrix} H_{\mathcal{I},\mathcal{I}} - A_{:,\mathcal{I}} \\ A_{:,\mathcal{I}}^T \end{bmatrix} \begin{pmatrix} \Delta x_{\mathcal{I}} \\ \Delta y \end{pmatrix} = - \begin{pmatrix} [\nabla x L(x_k^c, y_k^c, 0)]_{\mathcal{I}} \\ A^T x_k^c - b \end{pmatrix}$$

#### WHILE (not optimal) BEGIN

• Find  $\omega_k \searrow 0$  optimal solution  $x_k^c$  of

minimize 
$$\frac{1}{2}x^{T}Hx + g^{T}x - y^{T}(A^{T}x - b) + \frac{1}{2}\rho_{k}||A^{T}x - b||^{2}$$

- ② Find  $\mathcal{A}(x_k^c)$  & estimate penalty  $\bar{\rho} = 2 \|H_{\mathcal{I}}\| / \|A_{\mathcal{I}}A_{\mathcal{I}}^T\|$
- **3** IF  $\bar{\rho} > \rho_k$  THEN update  $\rho_{k+1} = \bar{\rho}$  & CYCLE ELSE update multiplier:  $y_k^c = y_k \rho_k (A^T x_k^c b)$
- Solve equality QP in subspace  $\rightarrow (\Delta x_{\mathcal{I}}, \Delta y)$

$$\begin{bmatrix} H_{\mathcal{I},\mathcal{I}} - A_{:,\mathcal{I}} \\ A_{:,\mathcal{I}}^{\mathsf{T}} \end{bmatrix} \begin{pmatrix} \Delta x_{\mathcal{I}} \\ \Delta y \end{pmatrix} = - \begin{pmatrix} [\nabla x L(x_{k}^{c}, y_{k}^{c}, 0)]_{\mathcal{I}} \\ A^{\mathsf{T}} x_{k}^{c} - b \end{pmatrix}$$

**5** Line-search on  $L(x_k^c + \alpha \Delta x, y_k^c + \alpha \Delta y, \rho)$ ; **update**  $x, y, k, \rho$ 

#### **END**

#### WHILE (not optimal) BEGIN

• Find  $\omega_k \searrow 0$  optimal solution  $x_k^c$  of

minimize 
$$\frac{1}{2}x^{T}Hx + g^{T}x - y^{T}(A^{T}x - b) + \frac{1}{2}\rho_{k}||A^{T}x - b||^{2}$$

- ② Find  $\mathcal{A}(x_k^c)$  & estimate penalty  $\bar{\rho} = 2 \|H_{\mathcal{I}}\| / \|A_{\mathcal{I}}A_{\mathcal{I}}^T\|$
- **3** IF  $\bar{\rho} > \rho_k$  THEN update  $\rho_{k+1} = \bar{\rho}$  & CYCLE ELSE update multiplier:  $y_k^c = y_k \rho_k (A^T x_k^c b)$
- Solve equality QP in subspace  $\rightarrow (\Delta x_{\mathcal{I}}, \Delta y)$

$$\begin{bmatrix} H_{\mathcal{I},\mathcal{I}} - A_{:,\mathcal{I}} \\ A_{:,\mathcal{I}}^{\mathsf{T}} \end{bmatrix} \begin{pmatrix} \Delta x_{\mathcal{I}} \\ \Delta y \end{pmatrix} = - \begin{pmatrix} [\nabla x L(x_{k}^{\mathsf{c}}, y_{k}^{\mathsf{c}}, 0)]_{\mathcal{I}} \\ A^{\mathsf{T}} x_{k}^{\mathsf{c}} - b \end{pmatrix}$$

**5** Line-search on  $L(x_k^c + \alpha \Delta x, y_k^c + \alpha \Delta y, \rho)$ ; **update**  $x, y, k, \rho$ 

#### **END**

1.-3. identify active set while 4. gives fast convergence

## Forcing Sequences of Augmented Lagrangian Methods

In general, two competing aims in augmented Lagrangian:

- reduce  $h_k := ||A^T x_k b|| \le \eta_k \searrow 0$

Note: QPPAL does not need  $\eta_k$ , see also [Dostal:99], [Delbos&Gilbert:03]



## Forcing Sequences of Augmented Lagrangian Methods

In general, two competing aims in augmented Lagrangian:

- reduce  $h_k := ||A^T x_k b|| \le \eta_k \searrow 0$
- 2 reduce  $\theta_k := \|\nabla L(x_k, y_k, \rho_k) z_k\| \le \omega_k \searrow 0$

Note: QPPAL does not need  $\eta_k$ , see also [Dostal:99], [Delbos&Gilbert:03]

... two arbitrary sequences,  $\eta_k, \omega_k$ 

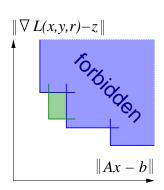
... why should one sequence  $\{\omega_k\}$ ,  $\{\eta_k\}$  fit all problems ???



#### Introduce a filter $\mathcal{F}$ for convergence

- list of pairs  $(\|A^Tx_I b\|, \|\nabla L_I z_I\|)$
- no pair dominates any other pair
- new  $x_k$  acceptable to filter  $\mathcal{F}$ , iff

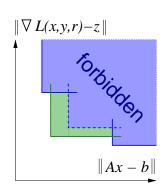
  - $\theta_k \leq 0.99 \cdot \theta_I \ \forall I \in \mathcal{F}$



#### Introduce a filter $\mathcal{F}$ for convergence

- list of pairs  $(\|A^Tx_I b\|, \|\nabla L_I z_I\|)$
- no pair dominates any other pair
- new  $x_k$  acceptable to filter  $\mathcal{F}$ , iff

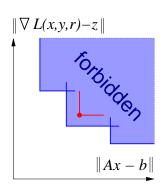
  - $\theta_k \leq 0.99 \cdot \theta_l \ \forall l \in \mathcal{F}$
- remove redundant entries



#### Introduce a filter $\mathcal{F}$ for convergence

- list of pairs  $(\|A^Tx_I b\|, \|\nabla L_I z_I\|)$
- no pair dominates any other pair
- new  $x_k$  acceptable to filter  $\mathcal{F}$ , iff

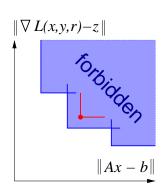
  - $\theta_k \leq 0.99 \cdot \theta_l \ \forall l \in \mathcal{F}$
- remove redundant entries
- reject new  $x_k$ , if  $h_k \ge h_l \& \theta_k \ge \theta_l$



#### Introduce a filter $\mathcal{F}$ for convergence

- list of pairs  $(\|A^Tx_I b\|, \|\nabla L_I z_I\|)$
- no pair dominates any other pair
- new  $x_k$  acceptable to filter  $\mathcal{F}$ , iff

  - $\theta_k \leq 0.99 \cdot \theta_I \ \forall I \in \mathcal{F}$
- remove redundant entries
- reject new  $x_k$ , if  $h_k \ge h_l \& \theta_k \ge \theta_l$



... an old friend from Chicago (Castellmarre di Stabia)



# Augmented Lagrangian Cauchy Pointe (Al Capone)

### Requirement on Cauchy Point $x_k^c$ for filter:

- ②  $\|\nabla L(x_k, y_k, \rho_k) z_k\| \le \omega_k$ ... optimality of Lagrangian



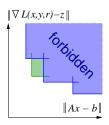


# Augmented Lagrangian Cauchy Pointe (Al Capone)

### Requirement on Cauchy Point $x_k^c$ for filter:

- ②  $\|\nabla L(x_k, y_k, \rho_k) z_k\| \le \omega_k$ ... optimality of Lagrangian

New: 
$$\omega_k := 0.1 \max \left\{ \| \nabla L_l - z_l \| \right\}$$
 ... depends on filter

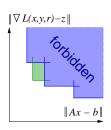


# Augmented Lagrangian Cauchy Pointe (Al Capone)

### Requirement on Cauchy Point $x_k^c$ for filter:

- ②  $\|\nabla L(x_k, y_k, \rho_k) z_k\| \le \omega_k$ ... optimality of Lagrangian

New: 
$$\omega_k := 0.1 \max \left\{ \| \nabla L_l - z_l \| \right\}$$
 ... depends on filter



#### Consequences of Filter

- ensures that back-tracking line-search will succeed ... if not acceptable then reduce  $\omega_{k+1} = \omega_k/2$
- **2** &  $\omega_{k+1} = \omega_k/2$  ensure can always find Al Capone

### A Filter for QPPAL

#### WHILE (not optimal) BEGIN

**1** Find  $\omega_k$  optimal solution  $x_k^c$  of

minimize 
$$\frac{1}{2}x^{T}Hx + g^{T}x - y^{T}(A^{T}x - b) + \frac{1}{2}\rho_{k}||A^{T}x - b||^{2}$$

- **②** Find  $\mathcal{A}(x_k^c)$  & estimate penalty  $\bar{\rho} = 2 \|H_{\mathcal{I}}\| / \|A_{\mathcal{I}}A_{\mathcal{I}}^T\|$
- **3** IF  $\bar{\rho} > \rho_k$  THEN update  $\rho_{k+1} = \bar{\rho}$  & CYCLE ELSE update multiplier:  $y_k^c = y_k \rho_k (A^T x_k^c b)$
- **5** Solve equality QP in subspace  $\rightarrow (\Delta x_{\mathcal{I}}, \Delta y)$

#### **END**

### A Filter for QPPAL

#### WHILE (not optimal) BEGIN

**1** Find  $\omega_k$  optimal solution  $x_k^c$  of

minimize 
$$\frac{1}{2}x^{T}Hx + g^{T}x - y^{T}(A^{T}x - b) + \frac{1}{2}\rho_{k}||A^{T}x - b||^{2}$$

- ② Find  $\mathcal{A}(x_k^c)$  & estimate penalty  $\bar{\rho} = 2 \|H_{\mathcal{I}}\|/\|A_{\mathcal{I}}A_{\mathcal{I}}^T\|$
- **3** IF  $\bar{\rho} > \rho_k$  THEN update  $\rho_{k+1} = \bar{\rho}$  & CYCLE ELSE update multiplier:  $y_k^c = y_k \rho_k (A^T x_k^c b)$
- **1** IF  $(x_k^c, y_k^c)$  not acceptable THEN  $\omega_{k+1} = \omega_k/2$  & CYCLE
- **5** Solve equality QP in subspace  $\rightarrow (\Delta x_{\mathcal{I}}, \Delta y)$
- Filter-search along  $(x_k^c + \alpha \Delta x, y_k^c + \alpha \Delta y)$ ; **update** x, y, k

#### **END**

### Properties of QPPAL

### Lemma (Friedlander)

First-order multiplier update & augmented system solve  $\Leftrightarrow$  Newton step on first order conditions  $(\nabla_x \mathcal{L}, \nabla_y \mathcal{L}) = 0$ 

## Properties of QPPAL

### Lemma (Friedlander)

First-order multiplier update & augmented system solve  $\Leftrightarrow$  Newton step on first order conditions  $(\nabla_x \mathcal{L}, \nabla_y \mathcal{L}) = 0$ 

Filter version has no restoration phase

- Step 4. IF  $(x_k^c, y_k^c)$  not acceptable THEN  $\omega_{k+1} = \omega_k/2$  & CYCLE
  - $\Rightarrow$  tighten tolerance of BCL  $\Rightarrow$  BCL is restoration phase
  - ⇒ always find Al Capone (Cauchy point)

### Properties of QPPAL

### Lemma (Friedlander)

First-order multiplier update & augmented system solve  $\Leftrightarrow$  Newton step on first order conditions  $(\nabla_x \mathcal{L}, \nabla_y \mathcal{L}) = 0$ 

#### Filter version has no restoration phase

- Step 4. IF  $(x_k^c, y_k^c)$  not acceptable THEN  $\omega_{k+1} = \omega_k/2$  & CYCLE
  - $\Rightarrow$  tighten tolerance of BCL  $\Rightarrow$  BCL is restoration phase
  - ⇒ always find Al Capone (Cauchy point)
- Augmented system solve is 2nd restoration phase:

$$A_{:,\mathcal{I}}x_{\mathcal{I}} = b - A_{:,\mathcal{A}}x_{\mathcal{A}}$$
 & full step  $\Rightarrow$  feasibility

### Outline

- Introduction and Motivation
- 2 Large-Scale Active-Set Methods for QP
  - Augmented Lagrangians for QPs
  - Filter Methods for Augmentd Lagrangian QPs
- 3 Large-Scale Active-Set Methods for NLP
  - Augmented Lagrangian Filter Method
  - Outline of Convergence Proof
  - Outlook and Conclusions



### Two-Phase Active-Set Framework for NLP

NLP: minimize 
$$f(x)$$
 subject to  $c(x) = 0, x \ge 0$ 

#### repeat

- Compute cheap first-order step  $x^{(k)} + s$ , e.g. LP/QP solve
- 2 Predict active set from s:  $A(x^{(k)} + s) \& I(x^{(k)} + s)$
- Ompute second-order EQP step on active set:

$$\begin{bmatrix} H_k & A_k \\ A_k^T \end{bmatrix} \begin{pmatrix} \Delta x \\ \Delta y \end{pmatrix} = \dots \qquad \text{Newton step}$$

where 
$$H_k = \nabla^2 L^{(k)}$$
 and  $A_k = \left[ \nabla c^{(k)} : I^{(k)} \right]$  active c/s

 $\textbf{ § Enforce global convergence \& set } \textit{k} \leftarrow \textit{k} + 1$ 

until optimal solution found

(Fletcher & de la Maza:89), (Gould & Robinson:10), (Fletcher:11)

Toward scalable nonlinear optimization

 $\Rightarrow$  replace LP/QP ... avoid pivoting, i.e. rank-one matrix updates

# Augmented Lagrangian Methods (LANCELOT)



### Augmented Lagrangian:

$$L_{\rho} := f(x) - y^{T} c(x) + \frac{\rho}{2} ||c(x)||_{2}^{2}$$
With sequences  $\omega_{k} \searrow 0$  and  $\eta_{k} \searrow 0$ 

#### repeat

- Find  $\omega_k$  optimal solution  $\hat{x}^{(k+1)}$  of minimize  $L_{\rho}(x, y^{(k)})$
- else if  $\|c(\hat{x}^{(k+1)})\| \leq \eta_k$  then update multipliers:  $y^{(k+1)} = y^{(k)} \rho_k c(\hat{x}^{(k+1)})$  else increase penalty:  $\rho_{k+1} = 2\rho_k$
- **3** Choose new  $(\eta_{k+1}, \omega_{k+1})$ ; set  $k \leftarrow k+1$  **until** (optimal solution found)

see e.g. (Conn, Gould & Toint:95) and (Friedlander, 2002)



## Augmented Lagrangian Methods (LANCELOT)

#### Advantage of Augmented Lagrangian Methods

• Scalable computational kernels

#### Disadvantages of Augmented Lagrangian Methods

- First-order method in multipliers ⇒ slow convergence
- 2 Arbitrary forcing sequences  $(\omega_k, \eta_k)$  ... one fits all NLPs?
- **3** Slow penalty update  $\Rightarrow$  slow for infeasible NLPs

#### Improving augmented Lagrangian methods:

- Add equality QP step for fast Newton-like convergence
- 2 Replace forcing sequence  $(\omega_k, \eta_k)$  by filter
- Exploit structure for penalty estimates & use restoration phase

Goal: extend (Friedlander & L., 2008) from QP to NLP

### Augmented Lagrangian Filter

Filter  $\mathcal{F}$  to replace forcing sequences  $(\omega_k, \eta_k)$ 

### Definition (Augmented Lagrangian Filter)

• Filter  $\mathcal{F}$  is a list of pairs  $(\eta(x), \omega(x, y))$  where

$$\omega(x,y) := \|\min\{x, \nabla_x L_0(x,y)\}\| \qquad \dots \text{ Lagrangian } L_0$$
 
$$\eta(x) := \|c(x)\| \qquad \dots \text{ constraint violation}$$

such that no pair dominates another

• A point  $(x^{(k)}, y^{(k)})$  acceptable to filter  $\mathcal{F}$  iff

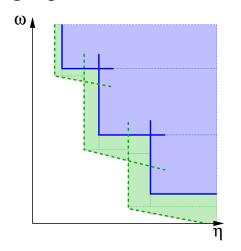
$$\eta(x^{(k)}) \le \beta \eta_l$$
 or  $\omega(x^{(k)}, y^{(k)}) \le \beta \omega_l - \gamma \eta(x^{(k)}), \quad \forall l \in \mathcal{F}$ 

Typically: 
$$\beta = 0.99, \ \gamma = 0.01$$

Approximate minimization of  $L_{\rho}(x, y^{(k)})$  until acceptable to filter



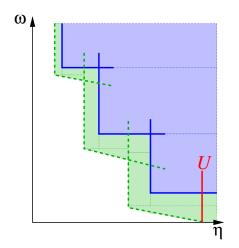
## Augmented Lagrangian Filter



• 
$$\omega(x, y) := \| \min\{x, \nabla_x L_0(x, y)\} \| \text{ and } \eta(x) := \| c(x) \|$$



## Augmented Lagrangian Filter



- $\omega(x, y) := \| \min\{x, \nabla_x L_0(x, y)\} \|$  and  $\eta(x) := \| c(x) \|$
- Automatic upper bound:  $U = \beta/\gamma \omega_{\text{max}}$ , because  $\omega \ge 0$

## Augmented Lagrangian Filter Method

```
while (x^{(k)}, y^{(k)}) not optimal do
    i=0; initialize \hat{x}^{(j)}=x^{(k)}, \hat{\omega}_i=\omega_k and \hat{\eta}_i=\eta_k
     repeat
          \hat{x}^{(j+1)} \leftarrow \text{approximate argmin}_{x>0} L_{\rho_k}(x, y^{(k)}) \text{ from } \hat{x}^{(j)}
          if restoration switching condition then
                Increase penalty: \rho_{k+1} = 2\rho_k & switch to restoration
                ... find acceptable (x^{(k+1)}, v^{(k+1)}) and set k = k+1
           end
           Provisionally update: \hat{y}^{(j+1)} = y^{(k)} - \rho_i c(\hat{x}^{(j+1)})
          Compute (\hat{\eta}_{i+1}, \hat{\omega}_{i+1}) and set j = j+1
     until (\hat{\eta}_i, \hat{\omega}_i) acceptable to \mathcal{F}_k;
     Set (x^{(k+1)}, y^{(k+1)}) = (\hat{x}^{(j)}, \hat{v}^{(j)})
     Get A^{(k+1)} = \{i : x_i^{(k+1)} = 0\} & solve equality QP
     if \eta_{k+1} > 0 then add (\eta_{k+1}, \omega_{k+1}) to \mathcal{F} ... set k = k+1;
end
```

# Approximate Minimization of Augmented Lagrangian

Inner initialization: j = 0 and  $\hat{x}^{(0)} = x^{(k)}$ 

For  $j=0,1,\ldots$  terminate augmented Lagrangian minimization,

$$\hat{x}^{(j+1)} \leftarrow \text{approximate argmin } L_{\rho_k}(x, y^{(k)})$$

when standard sufficient reduction holds:

$$\Delta L_{\rho_k} := L_{\rho_k}(\hat{x}^{(j)}, y^{(k)}) - L_{\rho_k}(\hat{x}^{(j+1)}, y^{(k)}) \ge \sigma \hat{\omega}_j \ge 0$$

E.g. Cauchy step on augmented Lagrangian for fixed  $\rho_k$  and  $y^{(k)}$ 

More natural than requiring reduction in F.O. error  $\hat{\omega}_j \searrow 0$ 



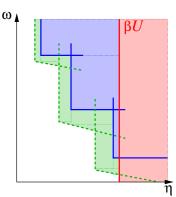
## Switching to Restoration

Goal: Infeasible NLPs  $\Rightarrow$  want to find minimize  $||c(x)||_2^2$  fast!

Switch to restoration, min ||c(x)||, if

- **1**  $\hat{\eta}_j \geq \beta U$  ... infeasible, or
- ②  $\hat{\eta}_j \ge M \min(1, \hat{\omega}_j^{\tau})$ , for  $\tau \in [1, 2]$  ... infeasible Fritz-John point, or

$$\eta_{\min} := \min_{I \in \mathcal{F}_L} \{ \eta_I \} > 0$$



### Lemma (Finite Return From Restoration)

 $\eta_l \ge \eta_{\min} \ \forall l \in \mathcal{F}_k \Rightarrow \exists \ x^{(k+1)}$  acceptable or restoration converges



## Second-Order Steps & KKT Solves

- $\mathbf{x}^{(k+1)} \leftarrow \underset{\mathbf{x} \geq 0}{\text{minimize}} \ L_{\rho}(\mathbf{x}, \mathbf{y}^{(k)}) \dots \text{ predicts } \mathcal{A}(\mathbf{x}^{(k+1)})$
- Accelerate convergence, by solving EQP with  $\Delta x_A = 0$ :

$$\begin{bmatrix} \tilde{H}_{k+1} & \tilde{A}_{k+1} \\ \tilde{A}_{k+1}^T \end{bmatrix} \begin{pmatrix} \Delta x_{\mathcal{I}} \\ \Delta y \end{pmatrix} = \begin{pmatrix} -\nabla f_{\mathcal{I}}^{(k+1)} \\ -c(x^{(k+1)}) \end{pmatrix}$$

where  $\tilde{H}_{k+1}$  is "reduced" Hessian wrt bounds  $(\Delta x_{\mathcal{A}} = 0)$ 

• Line-search:  $\alpha_{k+1} \in \{0\} \cup [\alpha_{\min}, 1]$  such that

$$(x^{(k+1)}, y^{(k+1)}) = (\hat{x}^{(k+1)}, \hat{y}^{(k+1)}) + \alpha_{k+1}(\Delta x^{(k+1)}, \Delta y^{(k+1)})$$

 $\mathcal{F}_k$ -acceptable

...  $\alpha_{k+1} = 0$  OK, because  $(\hat{x}^{(k+1)}, \hat{y}^{(k+1)})$  was acceptable



## Augmented Lagrangian Filter Method

```
while (x^{(k)}, y^{(k)}) not optimal do
    i=0; initialize \hat{x}^{(j)}=x^{(k)}, \hat{\omega}_i=\omega_k and \hat{\eta}_i=\eta_k
     repeat
          \hat{x}^{(j+1)} \leftarrow \text{approximate argmin}_{x>0} L_{\rho_k}(x, y^{(k)}) \text{ from } \hat{x}^{(j)}
          if restoration switching condition then
                Increase penalty: \rho_{k+1} = 2\rho_k & switch to restoration
                ... find acceptable (x^{(k+1)}, v^{(k+1)}) and set k = k+1
           end
           Provisionally update: \hat{y}^{(j+1)} = y^{(k)} - \rho_i c(\hat{x}^{(j+1)})
          Compute (\hat{\eta}_{i+1}, \hat{\omega}_{i+1}) and set j = j+1
     until (\hat{\eta}_i, \hat{\omega}_i) acceptable to \mathcal{F}_k;
     Set (x^{(k+1)}, y^{(k+1)}) = (\hat{x}^{(j)}, \hat{v}^{(j)})
     Get A^{(k+1)} = \{i : x_i^{(k+1)} = 0\} & solve equality QP
     if \eta_{k+1} > 0 then add (\eta_{k+1}, \omega_{k+1}) to \mathcal{F} ... set k = k+1;
end
```

## Overview of Convergence Proof

### Assumptions

- Functions f(x) and c(x) twice continuously differentiable
- $||c(x)|| \to \infty$  whenever  $||x|| \to \infty$  ... ignore EQP for analysis

### Outline of Convergence Proof

- Filter  $\mathcal{F}_k \Rightarrow$  iterates,  $x^{(k)}$  remain in compact set
- 2 Inner iteration is finite  $\Rightarrow \exists$  convergent subsequence
- **3** Mechanism of filter  $\Rightarrow$  limit points are feasible
- Show limit points are stationary in two cases:
  - Bounded penalty ... rely on filter
  - 2 Unbounded penalty ... classical augmented Lagrangian

#### Remark

Do not assume compactness, or bounded multipliers!

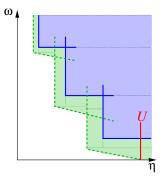
## Iterates Remain in Compact Set

### Lemma (All Iterates Remain in Compact Set)

All major and minor iterates,  $x^{(k)}$  and  $\hat{x}^{(j)}$  are in a compact set, C.

### Proof.

- Upper bound on filter  $(U = \beta/\gamma \omega_{\text{max}})$  $\Rightarrow \|c(x^{(k)})\| \leq U$  for all major iterates
- ② Switching condition  $(\hat{\eta}_j \leq \beta U)$  $\Rightarrow ||c(\hat{x}^{(j)})|| \leq U$  for all minor iterates
- Feasibility restoration minimizes ||c(x)|| $\Rightarrow ||c(x^{(k)})||$  bounded
- $\Rightarrow \|c(^{(k)})\| \leq U \text{ and } \|c(\hat{x}^{(j)})\| \leq U$



c(x) twice continuously differentiable &  $\|c(x)\| \to \infty$  if  $\|x\| \to \infty$ 

$$\Rightarrow x^{(k)}$$
,  $\hat{x}^{(j)} \in C$ , compact

### Finiteness of Inner Iteration

### Lemma (Finiteness of Inner Iteration)

The inner iteration is finite.

**Proof.** Assume inner iteration not finite  $\Rightarrow \exists \hat{x}^* = \lim \hat{x}^{(j)} \in C$ 

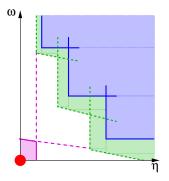
- **1** Fixed penalty:  $\rho_k \equiv \rho < \infty$
- ② Sufficient reduction of  $L_{\rho}(x, y^{(k)})$

$$\Rightarrow \Delta L_{\rho} \geq \sigma \hat{\omega}_{i}$$
; assume  $\hat{\omega}_{i} \geq \bar{\omega} > 0$ 

$$\Rightarrow L_{\rho}(\hat{x}^{(j)}, y^{(k)})$$
 unbounded

... but 
$$||c(\hat{x}^{(j)})||$$
,  $\rho$ , and  $f(x)$  bounded

- **3** Contradiction  $\Rightarrow \hat{\omega}_i \rightarrow 0$ , and  $\hat{\omega}_* = 0$
- **9** Switching:  $\hat{\eta}_i < M\hat{\omega}_i \Rightarrow \hat{\eta}_* \leq M\hat{\omega}_*$



 $\Rightarrow$   $(\hat{\eta}_*, \hat{\omega}_*) = (0, 0)$  and  $\exists$  filter acceptable points near (0, 0)

### Feasible Limit Points

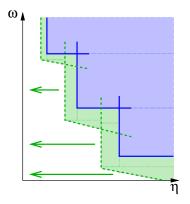
### Lemma (Feasible Limit Points)

In outer iteration, feasibility error  $\eta_k = ||c(x^{(k)})|| \to 0$ .

### Proof. Two cases:

- ②  $\eta_k > 0$ , subsequence  $\forall k \geq K_0$  see (Chin & Fletcher, 2003) ... envelope  $\Rightarrow \eta_k \rightarrow 0$

... standard filter argument



## First-Order Optimality

### Lemma (First-Order Stationarity)

First-order optimality  $\omega_k = \|\min\{x^{(k)}, \nabla_x L_0^{(k)}\}\| \to 0$ .

**Proof.** (1)  $\rho_k \leq \bar{\rho} < \infty$  and (2)  $\rho_k$  unbounded: classical proof

- Assume  $\omega_k \geq \bar{\omega} > 0$  & seek contradiction  $\Rightarrow \Delta L_{\bar{\rho}}^{in} = L_{\bar{\rho}}(x^{(k)}, y^{(k)}) L_{\bar{\rho}}(x^{(k+1)}, y^{(k)}) \geq \sigma \omega_k \geq \sigma \bar{\omega} > 0$
- First-order multiplier update,  $y^{(k+1)} = y^{(k)} \bar{\rho}c(x^{(k+1)})$

$$\Delta L_{\bar{\rho}}^{out} = L_{\bar{\rho}}(x^{(k)}, y^{(k)}) - L_{\bar{\rho}}(x^{(k+1)}, y^{(k+1)})$$

$$= \Delta L_{\bar{\rho}}^{in} - \bar{\rho} \|c(x^{(k+1)})\|_{2}^{2}$$

$$\geq \sigma \bar{\omega} - \rho \|c(x^{(k+1)})\|_{2}^{2}$$

• Feasible limit:  $c(x^{(k+1)}) \to 0 \Rightarrow \|c(x^{(k+1)})\|_2^2 \le \sigma \frac{\bar{\omega}}{2\rho}, \ \forall k \ge \bar{K}$  $\Rightarrow \Delta L_{\bar{\rho}}^{out} \ge \sigma \frac{\bar{\omega}}{2}, \ \forall k \ge \bar{K}$  outer iteration sufficient reduction

# First-Order Optimality (Proof cont.)

- Sufficient reduction at outer iterations:  $\Delta L_{\bar{\rho}}^{out} \ge \sigma_{\bar{2}}^{\bar{\omega}}$  $\Rightarrow L_{\bar{\rho}}(x,y) = f(x) - y^{T}c(x) + \frac{\rho}{2}\|c(x)\|_{2}^{2}$  unbounded
- $x^{(k)} \in C$  compact  $\Rightarrow f(x)$  and  $||c(x)||_2^2$  bounded
- Show  $y^T c(x) \leq M$  bounded:
  - Feasibility Lemma  $\Rightarrow \eta_k = \|c(x^{(k)})\| \to 0$
  - Filter acceptance: Monotone sub-sequences  $\eta_k \leq \beta \eta_{k-1}$
  - FO multiplier update:  $y^{(k)} = y^{(0)} \bar{\rho} \sum_{l} c^{(l)}$

$$\Rightarrow y^{(k)^{T}} c(x^{(k)}) = \left(y^{(0)} - \bar{\rho} \sum_{l} c^{(l)}\right)^{T} c^{(k)}$$

$$\leq \left(1 + \bar{\rho} \sum_{l} \eta_{l}\right) \eta_{k} \leq \eta_{0} \left(\beta^{k} + \bar{\rho} \sum_{l} \beta^{l+k}\right) \leq M$$

• Contradiction:  $L_{\bar{\rho}}(x,y) = f(x) - y^T c(x) + \frac{\rho}{2} ||c(x)||_2^2$  bounded  $\Rightarrow \omega_k \to 0$  ... first-order stationarity

## Key Computational Kernels

- lacksquare Filter stopping rule readily included in minimization of  $L_{
  ho}$ 
  - $\nabla L_{\rho}(\hat{x}^{(j+1)}, y^{(k)}) = \nabla L_{0}(\hat{x}^{(j+1)}, \hat{y}^{(j+1)}) = \hat{\omega}_{j+1}$
- Approximate minimization of augmented Lagrangian
  - projected gradient plus CG on subspace

$$\begin{aligned} \left[ H_k + \rho A_k A_k^T \right]_{\mathcal{I}, \mathcal{I}} \Delta x_{\mathcal{I}} &= -\nabla L_{\rho}(x^{(k)}, y^{(k)}) \\ \Leftrightarrow \left[ \tilde{A}_k^T - \rho^{-1} I \right] \begin{pmatrix} \Delta x_{\mathcal{I}} \\ u \end{pmatrix} &= \begin{pmatrix} -\nabla L_{\rho}(x^{(k)}, y^{(k)}) \\ 0 \end{pmatrix} \end{aligned}$$

- KKT system solve
  - $\bullet \ \left[ \begin{array}{c} \tilde{H}_k \ \tilde{A}_k \\ \tilde{A}_k^T \end{array} \right] \left( \begin{array}{c} \Delta x_{\mathcal{I}} \\ \Delta y \end{array} \right) = \dots$
  - indefinite reduced Hessian ⇒ inertia control
- $\Rightarrow$  exploit scalable matrix-free solvers based on  $H_k, A_k$

## Summary and Teaching Points

### Presented Active-Set Method for QP/NLP

- Augmented Lagrangian Filter for QP or NLP
  - Identify active set via augmented Lagrangian step
  - Perform EQP solve
  - Use filter instead of forcing sequences
- Main computational kernels are parallelizable
  - Bound-constrained optimization via projected-gradient with CG
  - KKT-system solves, using GMRES or MINRES